Multicritical and Crossover Phenomena in Surface Growth

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Extended scaling forms are usually required to account for the complex behavior near a multicritical point. We explore their role in understanding kinetic phase transitions described by the Kardar-Parisi-Zhang equation for interface growth. For a surface of dimension $d=2$, an exponentially slow logarithmic-to-power-law crossover is predicted from a renormalization-group analysis and compared with numerical simulations of a deposition and evaporation model. Derivation of scaling forms associated with the kinetic roughening transition at $d>2$ is presented.

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Study of the morphology of a moving interface is important for understanding and controlling many physical, chemical, and biological processes.[1-3] One such example is the growth of a thin film by random deposition.[4] Though the microscopic mechanisms which govern the growth and subsequent relaxation of the film are not yet entirely clear, it is generally recognized that noise in the deposition rate may induce a surface roughness which builds up from small to large length scales. This behavior is characterized by a scaling form for the mean-square surface width,

$$w^2(t,L) \sim L^{2\zeta} f(\xi(t)/L) . \quad (1)$$

Here ζ is the roughness exponent in the steady state, L is the linear size of the substrate, and $\xi(t) \sim t^{1/z}$ is a typical growing length scale up to which roughness has fully developed at time t. The scaling function $f(x)$ assumes a power law $x^{2\zeta}$ at $x \ll 1$ and approaches a constant at $x \gg 1$.

In certain physical situations, growth on sufficiently short distances (which translate to early times) follows a kinetics which is different from its asymptotic form (1). Such a situation is expected near a continuous morphological transition: The scaling of surface fluctuations is initially indistinguishable from its behavior at the transition, and it crosses over to the form (1) characterizing a single phase only at later times.[5] The transition between phases of different roughness and/or dynamic behavior usually bears a multicritical character; i.e., some or all phases involved exhibit critical fluctuations as well as at the transition. In analogy with equilibrium systems,[6] one may write down a multicritical finite-size scaling hypothesis

$$w^2(t,L) \sim L^{2\zeta_c} \mathcal{F}(t/L^{z_c}, h_1 L^{\phi_1}, h_2 L^{\phi_2}, \ldots) , \quad (2)$$

where ζ_c and z_c are the roughness and dynamic exponents at the (multicritical) transition point, h_i are the appropriate scaling fields[7] which vanish at the transition, and ϕ_i are the associated crossover exponents. Depending on the relative strength and sign of the scaling fields, a variety of asymptotic scaling forms of type (1) can be reached. For an *infinite* system the role of L is replaced by the growing length scale $\xi(t) \sim t^{1/z_c}$, and (2) reduces to

$$w^2(t) \sim t^{2\beta_c} \mathcal{G}(h_1 t^{\phi_1/z_c}, h_2 t^{\phi_2/z_c}, \ldots) , \quad (3)$$

where $\beta_c = \zeta_c / z_c$.

Recent numerical simulations on some growth models of *surface dimension* $d=2$ encountered a class of complex rescaling behavior[8-12] which occurs when the surface (i) grows out of a thermally rough phase under a sufficiently weak driving force, or (ii) is near a transition in the growth pattern from layerwise to continuous. Though the possibility of an extremely slow logarithmic-to-power-law crossover has been suggested,[13] the numerical data are prone to other ostensive interpretations, such as supporting an intermediate phase with no unique asymptotic scaling.[9] A similar controversy exists in interpreting results from simulations[10,14] of a continuum equation for surface growth proposed by Kardar, Parisi, and Zhang (KPZ).[13]

In this Letter we examine kinetic phase transitions described by the KPZ equation from the perspective of extended scaling hypothesis (2) and (3). We show in certain limits that explicit functional forms can be derived from a one-loop renormalization-group (RG) analysis. Our study reveals an exponentially slow logarithmic-to-power-law crossover at $d=2$. The results on the continuum equation are compared with a large-scale lattice simulation of a deposition and evaporation model. We present additional analytical results from the RG study which in particular produces a dimension-independent logarithmic scaling function at the roughening transition of the KPZ equation above $d=2$, whose form was conjectured previously based on numerical evidence.[11]

The KPZ equation for the local growth of surface height h takes the form[13]

$$\partial h/\partial t = \nu \nabla^2 h + (\lambda/2)(\nabla h)^2 + \eta(\mathbf{x},t) . \quad (4)$$

The Gaussian noise η is assumed to satisfy

$$\langle \eta(\mathbf{x},t)\eta(\mathbf{x}',t')\rangle = 2D\delta^d(\mathbf{x}-\mathbf{x}')\delta(t-t') .$$

In the absence of nonlinearity ($\lambda=0$) Eq. (4) can be solved exactly.[15] In particular, starting from a flat surface at $t=0$, the height-height correlation function in momentum space is given by

$$\langle h(\mathbf{k},t)h(\mathbf{k}',t)\rangle=(2\pi)^d\frac{D}{\nu k^2}(1-e^{-2\nu k^2 t})\delta^d(\mathbf{k}+\mathbf{k}') . \quad (5)$$

Summing over all momenta at $\mathbf{k}'=-\mathbf{k}$ yields

$$w^2(t,L)\simeq\int_{2\pi/L\le|\mathbf{k}|\le\pi/a}\frac{d^dk}{(2\pi)^d}\frac{D}{\nu k^2}(1-e^{-2\nu k^2 t}) , \quad (6)$$

where a is the smallest length scale of the problem. From (6) one obtains (1) with the "free-field" exponents $z_0=2$ and $\zeta_0=(2-d)/2$ (logarithmic roughness at $d=2$). In a mode-coupling scenario,[16] (5) is renormalized in the presence of nonlinearity through $\mathbf{k}$-dependent coefficients $\tilde{D}$ and $\tilde{\nu}$. The scaling property at $\lambda\neq0$ can then be derived from (6) using $\tilde{D}$ and $\tilde{\nu}$. This scheme is now considered in more detail in conjunction with a one-loop RG analysis.

Forster, Nelson, and Stephen[17] (FNS) developed a dynamic RG approach to Eq. (4). As usual, the nonlinear coupling is treated perturbatively from small to large length scales. Integrating over fluctuations on short distances renormalizes the "bare" coefficients ν_B, λ_B, and D_B to the effective ones $\tilde{\nu}$, $\tilde{\lambda}$, and $\tilde{D}$ at a new minimal length $\tilde{a}=ba$. The resulting RG flow equations are usually presented in terms of renormalized *and rescaled* variables

$$\nu=b^{z-2}\tilde{\nu},\quad \lambda=b^{\zeta+z-2}\tilde{\lambda},\quad D=b^{z-d-2\zeta}\tilde{D} \quad (7)$$

to facilitate discussion of fixed-point behavior. They were obtained by FNS in a one-loop approximation,[17]

$$d\nu/dl=[z-2+K_d g(2-d)/4d]\nu , \quad (8a)$$

$$d\lambda/dl=[\zeta+z-2]\lambda , \quad (8b)$$

$$dD/dl=[z-d-2\zeta+K_d g/4]D , \quad (8c)$$

which are valid when the dimensionless coupling parameter $g\equiv(a/\pi)^{2-d}D\lambda^2/\nu^3$ is sufficiently small (weak coupling). Here $K_d^{-1}=2^{d-1}\pi^{d/2}\Gamma(d/2)$, and $l=\ln b$. The Galilean invariance of (4) gives $\tilde{\lambda}=\lambda_B$ which has no scale dependence.[13]

Figure 1 illustrates the phase diagram of the KPZ

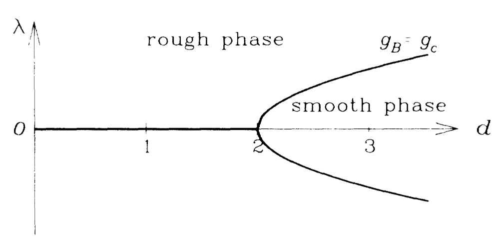

FIG. 1. Schematic phase diagram of the KPZ equation from the one-loop RG analysis. Transitions are marked by thick lines.

equation in terms of the nonlinear parameter λ, whose strength and sign can often be controlled.[18] It is obtained from the combined flow equation

$$\frac{dg}{dl}=(2-d)g+K_d\frac{2d-3}{2d}g^2+O(g^3) , \quad (9)$$

which has two fixed points at $g_0=0$ and $g_c=2d(d-2)K_d^{-1}/(2d-3)$. For $d\equiv2+\epsilon>2$, there is a smooth phase associated with the stable fixed point g_0. A transition into a (presumably) rough phase occurs as g is increased beyond the unstable fixed point $g_c\sim\epsilon$. The exponents at the transition are known to first order in ϵ, $\zeta_c=O(\epsilon^2)$, $z_c=2+O(\epsilon^2)$. At $d=2$ the two fixed points collapse and both become marginally unstable. For $d\le2$ a transition occurs at $\lambda=0$ (unstable fixed point g_0) between two rough phases of identical exponents.

The scaling property (1) is a direct consequence of scale invariance of (4) under a simultaneous transformation $\mathbf{r}\to b\mathbf{r}$, $t\to b^z t$, $h\to b^\zeta h$ and (7) at a fixed point of the RG flow.[13] It also follows from (6) if D and ν in the expression are replaced by the effective coefficients $\tilde{D}(b)$ and $\tilde{\nu}(b)$, with $b\sim k^{-1}$. The latter scheme may be justified within the one-loop perturbative approach.[13,17,19] We analyzed the crossover behavior of the RG flow defined by (8) for $d\ge2$. It follows from (8a) that, in the smooth phase, and around the transition $g_c\sim\epsilon$, ν_B is not renormalized (to the first order in ϵ). We now discuss results for the mean-square surface width obtained from the renormalization of D_B. Details of the calculation will be presented elsewhere.

(a) $d=2$.—Integrating (9) and (8c) at $\zeta_0=0$, $z_0=2$ gives

$$\tilde{D}(b)\simeq\frac{D_B(\ln\xi_c)}{\ln(\xi_c/b)} , \quad (10)$$

where $\xi_c=\exp(8\pi/g_B)$ is the crossover length in units of a, and $g_B=(a/\pi)^{2-d}D_B\lambda_B^2/\nu_B^3$. Following the procedure outlined above, we obtain, for an infinite system,

$$w^2(t)\simeq\frac{D_B\ln\xi_c}{\pi\nu_B}\ln\frac{\ln\xi_c}{\ln\xi_c/\xi(t)} , \quad (11)$$

which is valid when the growing length scale $\xi(t)\simeq\xi_0 t^{1/z_0}$ is small compared to ξ_c. The logarithmic roughness at $\lambda=0$ is recovered in the limit $\xi_c\to\infty$. The singularity of (11) at $\xi(t)=\xi_c$ is due to lack of a strong-coupling fixed point of (9) at a finite g. It can be removed by connecting (11) to the asymptotic form (1), taking ξ_c to be the unit of length and $\ln\xi_c$ the renormalized amplitude,

$$w^2(t)\simeq\frac{D_B\ln\xi_c}{\pi\nu_B}\left[G\left(\frac{\xi_0 t^{1/z_0}}{\xi_c}\right)+\ln\ln\xi_c\right] , \quad (12)$$

where $G(x)\simeq-\ln(-\ln x)$ at $x\ll1$ and $\sim x^{2\beta z_0}$ at $x\gg1$. We expect (12) to cover the whole crossover regime of the KPZ equation, though the explicit form of G is known (from the one-loop calculation) only when its argument is sufficiently small. The steady-state surface width of a finite system satisfies a scaling similar to (12), with the argument of G replaced by L/ξ_c. Choosing g_B as the scaling field, the one-loop calculation yields a crossover exponent $\phi=0$. The crossover from the logarithmic to a power-law scaling is thus *exponentially slow*; e.g., reducing g_B from 10 to 1 brings ξ_c from about 10 to about 10^{11}, a change of ten decades in the crossover length.

(b) $d>2$.—In this case

$$\frac{\tilde{D}(b)}{D_B} \simeq \begin{cases} (1+\xi_c^\epsilon)/[1+(\xi_c/b)^\epsilon], & g_B<g_c, \quad (13a) \\ b^\epsilon, & g_B=g_c, \quad (13b) \\ (\xi_c^\epsilon-1)/[(\xi_c/b)^\epsilon-1], & g_B>g_c. \quad (13c) \end{cases}$$

Here $\xi_c \simeq |1-g_c/g_B|^{-1/\epsilon}$. Like (10), (13c) is valid only when b is sufficiently smaller than ξ_c.

At the transition $g_B=g_c$, the power-law behavior of $\tilde{D}(b)$ yields a *dimension-independent* scaling form $w^2(t,L) \sim \ln[L\tilde{F}(t/L^2)]$, conjectured previously on the basis of a numerical study.[11] From (6) one obtains $\ln\tilde{F}$ explicitly in terms of an exponential integral. In our calculation the logarithmic scaling at the transition is only an order-ϵ result, but its validity resides merely in $z_c=2$ being exact.[20] Sufficiently close to the transition, fluctuations on length scales much less than ξ_c are still logarithmic, but now the crossover is more rapid than in the $d=2$ case. For $L \gg \xi_c$ and $t \gg \xi_c^{z_c}$, our calculation shows that $w^2(t,L)$ saturates to a finite value $w_R^2 \simeq D_B(\pi\nu_B)^{-1}\ln\xi_c$ on the smooth side of the transition. On the rough side $w^2(t,L)$ should presumably cross over to a power law (1) as observed in numerical studies.[9,11] Explicit crossover scaling functions can be readily derived as in the previous case. Identifying g_B-g_c with the scaling field in (2), the crossover exponent is found to be $\phi=\epsilon$.

In the following we compare the predicted scaling (12) with numerical-simulation data on the hypercube-stacking model[11] at $d=2$. This is a solid-on-solid model for the (111) surface of a simple-cubic structure. Growth is controlled by deposition and evaporation of particles at eligible sites with rates p^+ and p^-, respectively. Sublattice updating scheme and periodic boundary conditions are adopted for simulations in a strip geometry. Time is measured in units of sweeps of the whole surface. As reported previously,[11] at a fixed $p^+=\frac{1}{2}$, the model exhibits a logarithmic scaling at $p^-=\frac{1}{2}$ and a power-law one at $p^-=0$. Crossover is expected to occur at intermediate values of p^-, with a crossover length ξ_c which diverges as $p^- \to p^+$.

We studied a system of $N=L^2=5760^2$ surface sites at $p^+=\frac{1}{2}$ with a varying p^-. Saturation of the surface width at this size is estimated to take place at $t \gtrsim 5\times10^5$. Because of the difficulty in exploring the whole crossover regime from a single run at a p^- very close to p^+, we have instead performed a number of simulations up to $t=4096$ at different values of p^-. Each set of data should then fit part of the scaling curve (12) with its own crossover length $\xi_c(p^-)$ and prefactor of the scaling function $A(p^-)$. To facilitate the comparison we plotted $w^2(2t)-w^2(t)$ vs t on a log-log scale, as shown in Fig. 2. In this way the time-independent term in (12) (as well as possible intrinsic width of the surface) drops out. In addition, a logarithmic $w^2(t)$ is represented by a constant on the plot, while a power-law behavior has the usual appearance of a straight line at a finite slope. A data collapse for $\frac{1}{16} \le p^- \le \frac{3}{16}$ is achieved through a horizontal and vertical translation of each data set at $t \ge 4$ (shown in the inset) by an amount $2\log_{10}\xi_c(p^-)$ and $\log_{10}A(p^-)$, respectively. This fitting procedure becomes ambiguous when the curvature of a data set becomes too small, which is the case at larger values of p^-. The solid line represents the one-loop result for $G(\sqrt{2u})-G(\sqrt{u}) \simeq -\ln(1+\ln2/\ln u)$ at small $u=\xi^2(t)/\xi_c^2 \sim t/\xi_c^2$ (also shifted). The dashed line indicates an asymptotic power-law dependence with $\beta=0.24$.[11] We conclude from Fig. 2 that the seemingly decreasing effective exponent $\beta_{\rm eff}$ with increasing p^- (at least up to $p^-=\frac{3}{16}$) can be interpreted as due to a crossover effect. Furthermore, the data-collapse curve gives a numerically determined form for the scaling function G which matches well with the solid line at small values of the scaling variable. We interpret deviations of the early-time data at $p^-=\frac{3}{16}$ from the analytic curve as due to transient effects not described by the continuum equation. Such effects may arise due to, e.g., discrete-time dynamics adopted here and the underlying lattice structure.

A further check on the scaling form (12) can be made by analyzing the dependence of A on ξ_c. In Fig. 3 we plotted ξ_c and A obtained above on a semilogarithmic scale. The rapid increase of ξ_c with decreasing

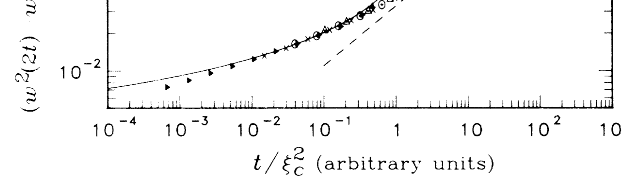

FIG. 2. Scaled surface width data vs time showing data collapse at $p^+=\frac{1}{2}$ and various values of p^- (given in the inset). The solid line shows the predicted behavior from the one-loop RG analysis. The dashed line gives the asymptotic power law at $\beta=0.24$. Inset: Unscaled data on the same scale.

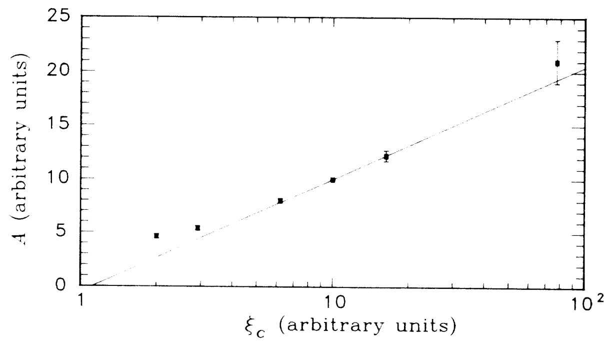

FIG. 3. Crossover length ξ_c vs scaling amplitude A. Relative error bars on ξ_c (not shown) are comparable to those on A.

$\kappa=(p^+-p^-)/p^+$ is evident: A 30% decrease in κ increases ξ_c by more than 30 times. The straight line in the figure gives the dependence of A on ξ_c assuming D_B/v_B to be a constant. Our data thus show that D_B/v_B depends only weakly on p^-.[21] It would be interesting to study this dependence in more detail and to verify the predicted exponential law $\xi_c \sim \exp(8\pi/g_B)$ by measuring the bare parameters.

In summary, we have demonstrated the importance of multicritical scaling in analyzing kinetic phase transitions. We discussed in detail the crossover from logarithmic to power-law scaling which occurs in the weak-coupling regime of the KPZ equation at $d=2$ and above the roughening transition at $d>2$. Explicit scaling forms in various limits were obtained through a one-loop RG analysis. By employing extended scaling forms we established that the observed varying effective exponent in a large-scale simulation of a deposition and evaporation model is due to an exponentially slow crossover of the KPZ equation at $d=2$. Our results may shed some light onto the recent controversy over the nature of kinetic phase transitions(s) in various (2+1)-dimensional growth models. Given the ineffectiveness of the nonlinear term in driving the system into the strong-coupling regime at $d=2$, it would be interesting to explore the effect of adding other terms to the continuum KPZ equation, which may modify the crossover behavior or even the phase diagram discussed here.

Very recently, Guo, Grossmann, and Grant[22] proposed a crossover scaling form connecting logarithmic to power-law roughness in (2+1) dimensions, parametrized by a crossover exponent $\phi'=z_c/\phi$. From the simulation they obtained $\phi'\simeq 4.5$. Our scaling form (12) corresponds to a suitable $\phi'\rightarrow\infty$ limit of their form. We note that any finite value of ϕ' is inconsistent with the perturbative RG scheme of FNS.

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